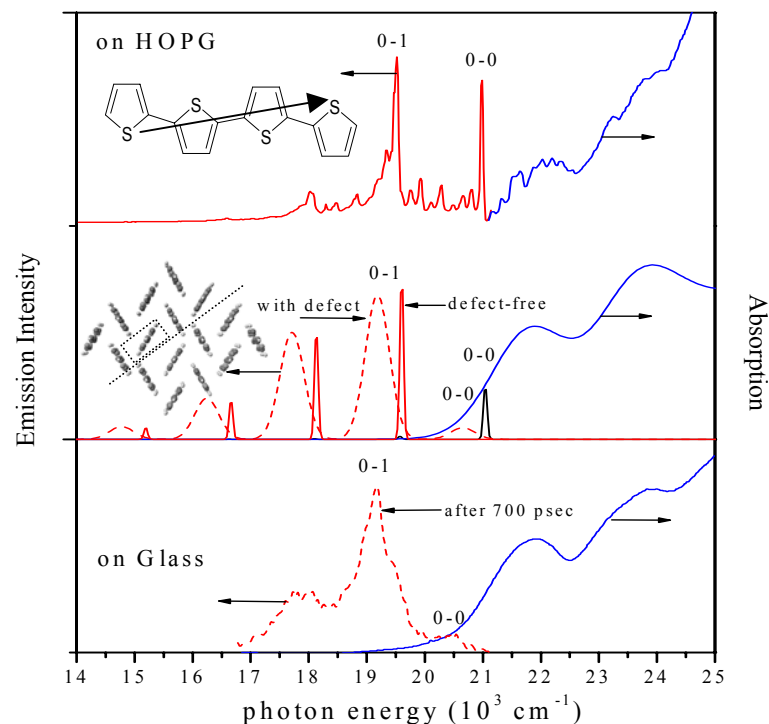


# Optical Excitations in Conjugated Oligomer and Polymer Aggregates: A Computational Approach

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Thin films of  $\pi$ -conjugated organic molecules, from relatively small oligomers to their parent polymers, are receiving widespread attention as semiconductors in applications such as flat-panel displays, electronic labels and even solid-state lighting. However, despite all of the experiments devoted to organic thin films, there remains much that is unknown regarding the basic theory of how they conduct charge or interact with light. Our work is dedicated to understanding in a fundamental way how light is absorbed and emitted in molecular aggregates and films of  $\pi$ -conjugated oligomers and polymers. The photophysics is affected by several important processes such as the electronic coupling between molecules, the coupling between electronic transitions and molecular vibrations, and the presence of structural and point defects.



Calculated absorption and emission spectra for defected and defect-free  $\alpha\text{T4}$  films (middle panel) compared to experimental spectra on graphite (top) and glass (bottom) substrates.